Construction of Numerical Tools to Improve Predictability & Reliability of Compressible Turbulence Simulations

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TTT-RCA CFD Prediction Error Assessment Workshop

March 20-22, 2018, Lockheed-Martin Center for Innovation

Outline

- Objective
- Technical Challenge
- Approach
- Results
- Summary

NASA TTT/RCA Support: Less than one full time support

Research results accomplished today cannot be achieved without leveraging DOE grants & outside no-cost collaborators

Objectives

Selected Research to be Presented Today:

Improve Nonlinear Stability, Accuracy & Correct Shock Speeds of High Order Methods for Compressible Turbulence

Remarks:

- Accurate methods for rapidly developing flows might not be accurate/stable enough for long time integration of turbulent flows
- Straightforward pointwise evaluation of source terms might produce wrong physical solutions (e.g., using methods developed for non-reacting/combustion flows)
- Solutions of the discretized counterparts but NOT solutions of the chosen governing equation:
  - Numerical chaos/turbulence & false prediction of laminar transition to turbulence can be obtained
  - Misleading Conclusion: Results in literature indicating certain chosen governing equation flows exhibit Chaotic/Turbulent behavior by merely analyzing the computed data (e.g., time series analysis or shallowing lemma techniques of the computed data)

Challenges in Numerical Method Development

(Multiscale DNS & LES, and Aeroacoustics Turbulence Applications)

- **Accurate schemes developed for short time integration might suffer from nonlinear instability for longer time integration**
- **Numerical stability & accuracy requirements are an intricate balancing act**
  - > More stable schemes usually contain more numerical dissipation than their higher accuracy counterparts
  - > Turbulence cannot tolerate numerical dissipation
  - > Proper amount of numerical dissipation is required for stability in the vicinity of discontinuities
  - > Reacting/combustion flows containing stiff source terms:
    - Numerical dissipation & under-resolved grid may lead to incorrect shock speed
    - Need well-balanced schemes to preserved certain physical steady states exactly
- **DNS & LES of turbulent flows containing shock-free turbulence, strong shocks & high gradient/shocklets during different stages of the computational time evolution cannot be solved accurately with standard numerical method construction**
- **Forced compressible turbulence can initially start with shock-free turbulence but might develop into flows with moderate to strong shock waves at a later time evolution** (Kotov et al. JCP, 2016)

Stable & Accurate Temporal & Spatial Low Dissipative & Dispersive methods applicable to long time integration are required

(Yee & Sjogreen, 2007-2017, Sjogreen & Yee, 2016-2017, Wang et al., 2009-2015, Kotov et al., 2011-2016)

Numerical Example

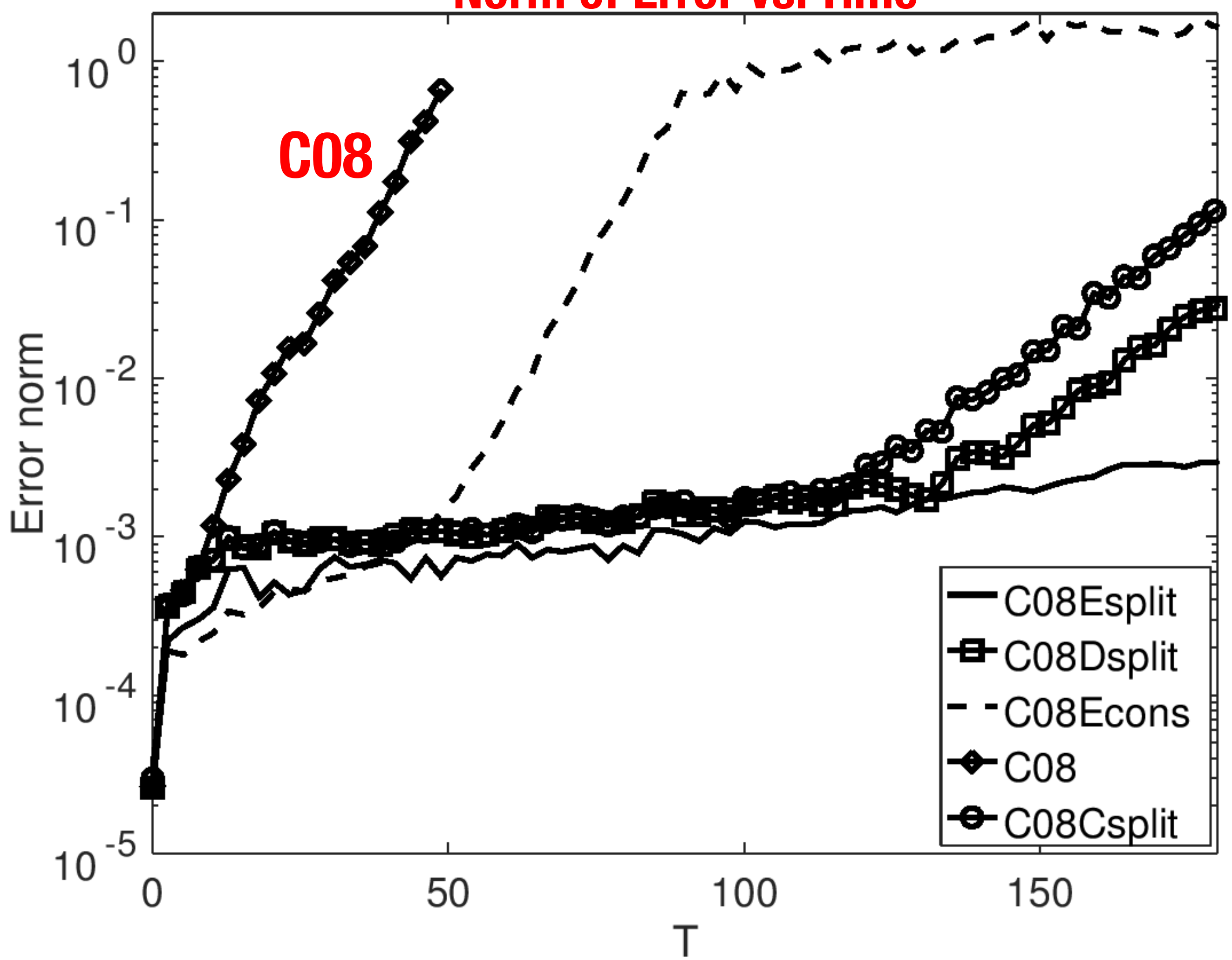
Long Time Integration of Smooth Flows

Accurate schemes developed for short time integration might suffer from nonlinear instability for longer time integration

2D Isentropic Vortex Convection

Translation of initial data exactly if no numerical dissipation added
8^{th} order central (C08) vs. 4 different 8^{th}-order skew-symmetric splittings

Norm of Error vs. Time



Improve numerical stability for longer time integrations via
4 skew-symmetric splittings of the inviscid flux derivative before the application of non-dissipative high order central schemes
(different accuracy)

Numerical Examples

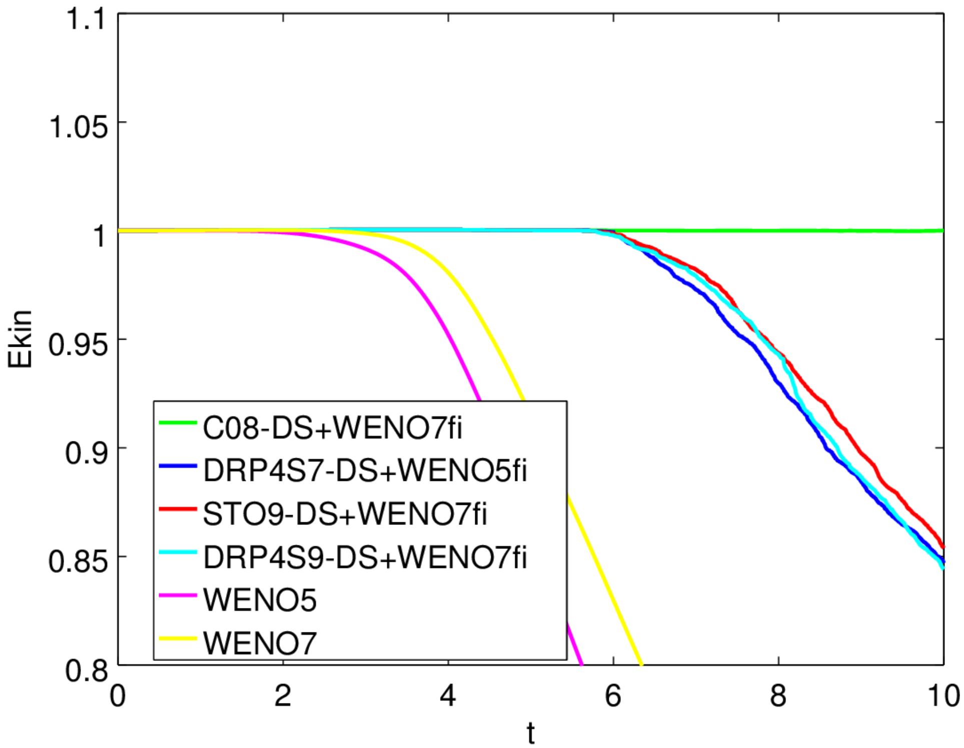
3D DNS Computations of Smooth Flows & Turbulence with Discontinuities

- **Standard shock-capturing methods are too diffusive for long time integration**
- **Careful design of added appropriate nonlinear numerical dissipations can improve accuracy**

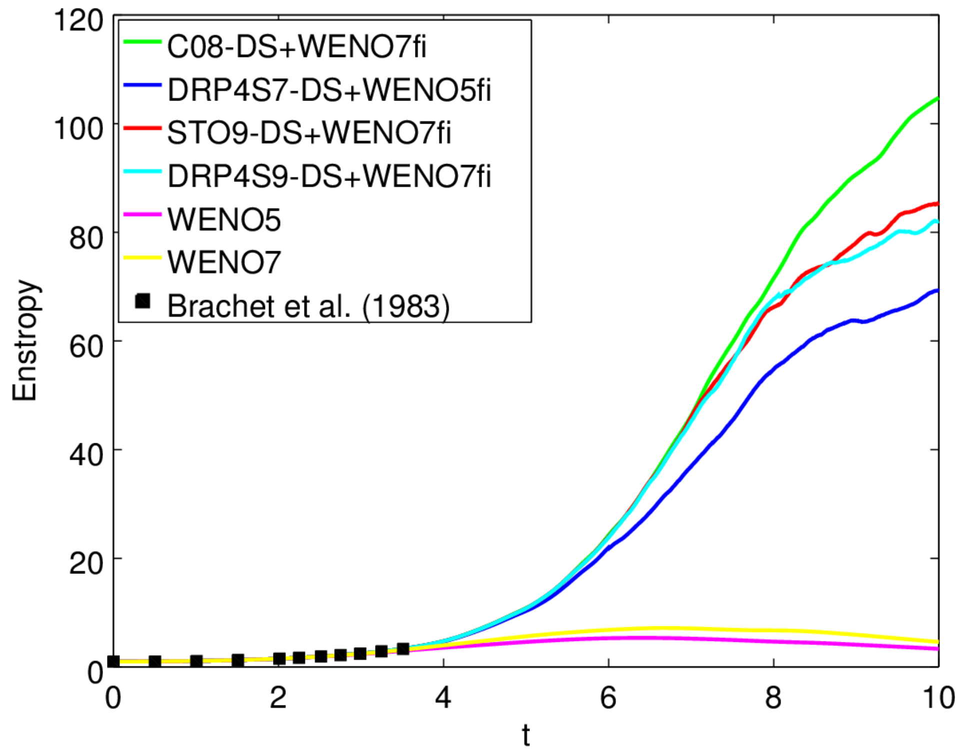
3D Taylor-Green Vortex (Compressible & Inviscid)

(Comparison of 6 Methods, 64^3 grids)

Kinetic Energy



Enstrophy



C08-DS+WENO7fi: 8^{th}-order central + Ducros et al. split +WENO7fi

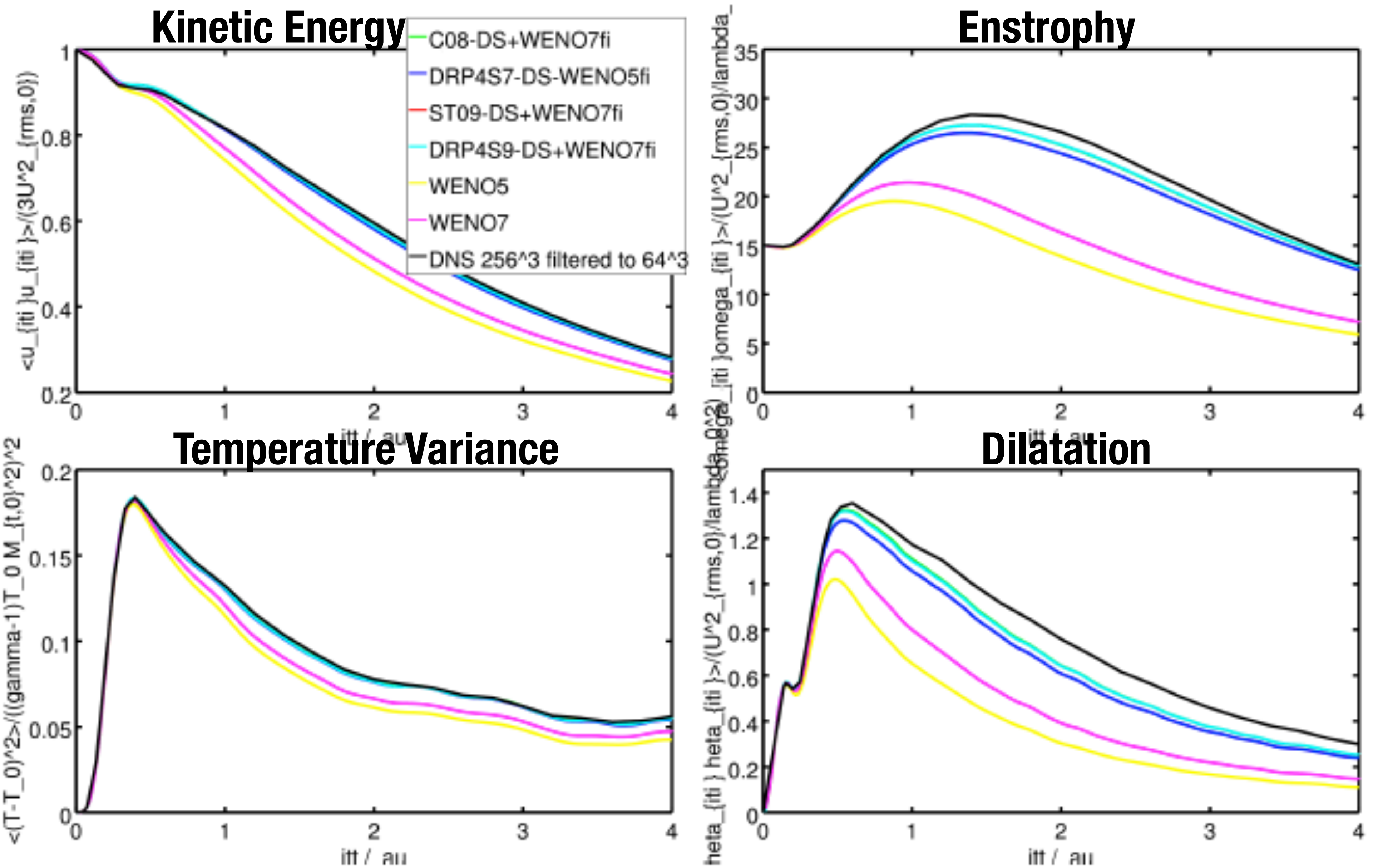
DRP4S7-DS+WENO5fi: Tam & Webb 4^{th}-order DRP, 7pt grid stencil + Ducros et al. split +WENO5fi

ST09-DS+WENO7fi: Bogey & Bailly 4^{th}-order DRP, 9pt grid stencil + Ducros et al. split +WENO7fi

DRP4S9-DS+WENO7fi: Tam & Webb 4^{th}-order DRP, 9pt grid stencil + Ducros et al. split +WENO7fi

3D Isotropic Turbulence with Shocklets

(Comparison of 6 Methods, 64^3 grids)



Spurious Numerics Due to Source Terms

Source Terms: Hyperbolic conservation laws with source terms – Balanced Law

> Most high order shock-capturing schemes are not well-balanced schemes

> High order WENO/Roe & their nonlinear filter counterparts are well-balanced for certain reacting flows – Wang et al. JCP papers (2010, 2011)

Stiff Source Terms:

> Numerical dissipation can result in wrong propagation speed of discontinuities for under-resolved grids if the source term is stiff (LeVeque & Yee, 1990)

> This numerical issue has attracted much attention in the literature – last 27 years (Improvement can be obtained easily for a single reacting flow case)

> A New Sub-Cell Resolution Method has been developed for stiff systems on coarse mesh (Wang et al., JCP, 2012 ; CiCP 2016)

Nonlinear Source Terms:

> Occurrence of spurious steady-state & discrete standing-wave numerical solutions -- due to fixed grid spacings & time steps (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990 – 2002)

Stiff Nonlinear Source Terms with Discontinuities:

> More Complex Spurious Behavior
> Numerical combustion, certain terms in turbulence modeling & reacting flows

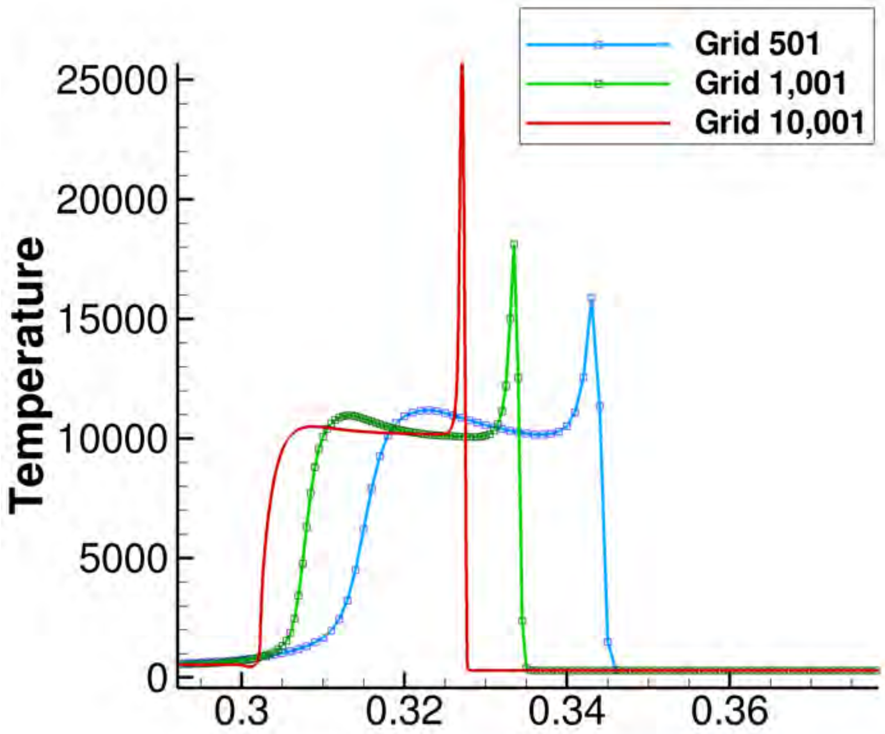
Stiff Source Terms: Wrong Discontinuity Locations

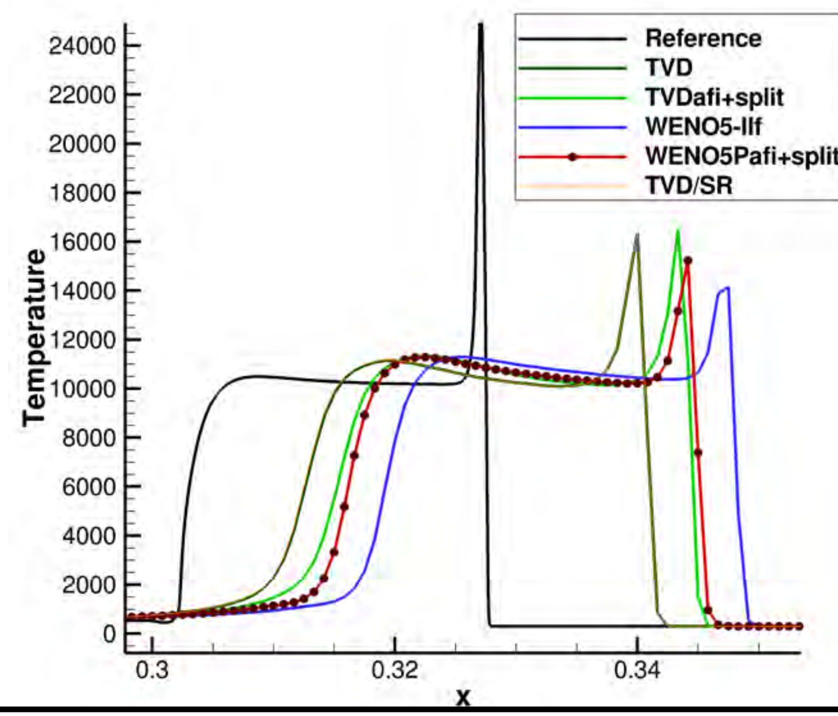
(Grid & method dependence of shock & shear locations)

TACP - Transformational Tools & Technologies Project

NASA *Electric Arc Shock Tube* (EAST)

- 1D Computation: 13 species(Air+He) using MUTATION library; L = 8.5 m
- Fine grid step h = 0.05mm, 16 times finer than coarse grid





Note: Problems without stiff source term - Grid size & conservative schemes used DO NOT affect locations of discontinuities

Implication: The danger in trusting numerical simulation for problems with stiff source terms

Non-standard behavior observed in non-reacting flows (Yee et al. JCP, 2014; Kotov et al. JCP, 2015)

Approach

- Schemes that mimic the property of the chosen governing equations
- Schemes that preserve key physical properties
- Schemes that are high order, low dissipation & low dispersive error suitable for a wide range of flow speeds (require local flow sensors to adaptively minimize the dissipation and dispersion errors)
- Schemes that are stable, efficient & highly parallelizable
- Schemes with high order stable discrete numerical boundary operators
- Schemes that are applicable for DNS & LES in 3D curvilinear spatial & time varying deforming grids
- Quantification of numerical uncertainty via dynamical numerical analysis – A nonlinear approach

Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al. and Kotov et al. (1999-2017)

Methods to Improve Nonlinear Stability & Accuracy

(Long Time Wave Propagation & Long Time Integration of Compressible Fluids & Plasma)

- **Skew-Symmetric Splitting** of the inviscid flux derivative before the application of non-dissipative centered schemes
- **DRP** (Dispersion Preservation-Relation) schemes as **alternatives** to splitted version of classical high order central schemes
- **High-Order Entropy Conservative Numerical Fluxes** with Entropy Satisfying Properties - Numerical solution satisfies an additional discretized conservation law
- Standard high order **Linear Filters** are to be **replaced by** high order **Nonlinear Filters** Yee et al., Yee & Sjogreen, Sjogreen & Yee, Kotov et al. (1999-2017)
- **Smart Flow Sensors** to provide locations & amount of needed numerical dissipation Yee & Sjogreen, Kotov et al. (2009-2016)
- **Nonlinear Dynamics** is utilized to complement the traditional linearized stability theory (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, Wang et al., Kotov et al. 1990- 2015)
  - Minimize numerically induced false transition to turbulence
  - Minimize numerical instability due to long time integration of turbulent flows
  - Minimize numerically induced standing wave solutions
  - Minimize wrong shock speeds

Yee et al. high-order nonlinear filter schemes with smart local flow sensors

Skew-Symmetric Splitting of Inviscid Flux Derivatives
(Improve nonlinear stability for high order central schemes)

Olsson & Oliger 1994, Yee et al. 1999, Ducros et al. 2000, Pirozzoli 2009, Sjogreen et al. 2017

- **Entropy splitting:** Semi-conservative splitting for shock-free turbulence
  (Olsson & Oliger 1994, Yee et al. 1999-2007, Sandham et al. 2002-present)
- **Natural Splitting:** Linearized Euler & Non-conservative Systems
- **Splitting to Preserve Discrete Momentum and/or Energy Conservation:**
  (Arakawa 1966, Blaisdell et al. 1996, Mansour 1980, etc.)
- **Ducros et al. Type Conservative Splitting:** Euler & MHD (Sjogreen et al. 2017)
- **Generalized Skew-Symmetric Splitting:** 3-parameter family (Pirozzoli 2009)

Preprocessing Step: Improve stability of classical central scheme

Replacing high order classical central approximation of the inviscid flux derivative
➔ High order approximation of their split form counterpart

High Order Entropy Conservative Methods

(One way to improve nonlinear stability & minimize added numerical dissipation)

- **Numerical solutions satisfy additional discretized conservation law**
- **Low order entropy conservative methods with linear numerical dissipation for shock-capturing require further accuracy improvement**
  (Tadmor 1984 – gas dynamics; Janhunen 2000 – MHD; Winters & Gassner 2016 – MHD)
- **High order entropy conservative methods for central schemes**
  (Fjordholm et al. 2012 – ENO; Sjogreen & Yee 2016, 2017– central + nonlinear filter, gas dynamics & MHD)

Plasma (Hypersonic Flows):

Four forms of the MHD equations to be considered

> Conservative form
> Godunov/Powell symmetrizable form (non-conservative)
> Janhunen form: (Div B) terms not included in the gas dynamics part of the equations)
> Brackbill & Barnes form

Three forms of the entropy fluxes to be considered

Winter & Gassner 2016, Chandrasheka & Klingenbery 2016, Sjogreen & Yee 2016-2017

Well-Balanced High Order Nonliner Filter Schemes
Non-Reacting & Reacting Flows

Yee et al., *1999-2017, Sjogreen &Yee, 2004-2017,* **Wang et al.**, *2009-2010. Kotov et al., 2012-2016*

Preprocessing step

Condition (equivalent form) the governing equations by, e.g., *Yee et al. Entropy Splitting & Ducros et al. Splitting* to improve numerical stability

High order low dissipative base scheme step (Full time step)

- High order **Central, DRP, or Entropy Conser. Num. Flux** scheme
- SBP numerical boundary closure, matching spatial & temporal order conservative metric evaluation *Vinokur & Yee, Sjögreen & Yee, Yee & Vinokur* (2000-2014)

Nonlinear filter step

- Filter the base scheme step solution by a dissipative portion of **any** positive high-order shock capturing scheme, e.g., **7^{th}-order positive WENO**
- Use local flow sensor to control the amount & location of the nonlinear numerical dissipation to be employed

Well-balanced scheme: preserve certain non-trivial physical steady state solutions of reactive eqns exactly

Note: "Nonlinear Filter Schemes" not to be confused with "LES filter operation"

Numerical Examples of Improved Nonlinear Stability & Accuracy by New Approach

Selected Illustrations:

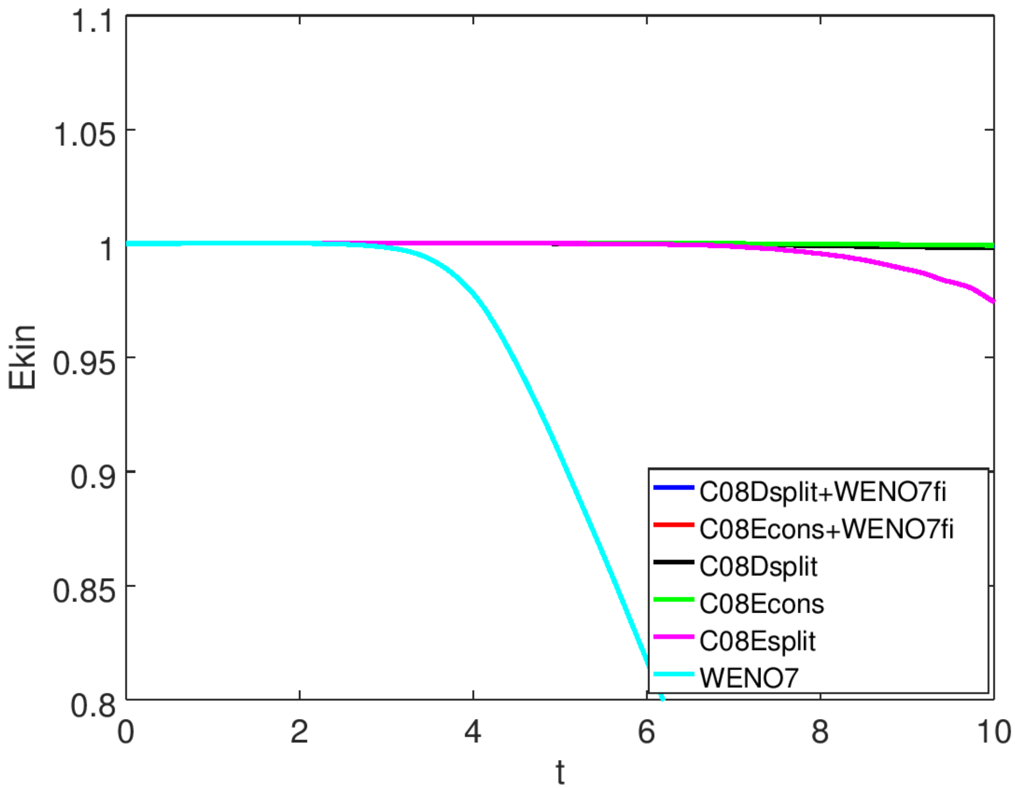
3D DNS Taylor & Green and Isotropic Turbulence

More Complicated 3D Flows & LES:

Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al. and Kotov et al. (1999-2017)

3D Taylor-Green Vortex (Compressible & Inviscid)
(Skew-Symmetric Splitting vs. Entropy Conservative Methods, 64^3 grids)

Kinetic Energy



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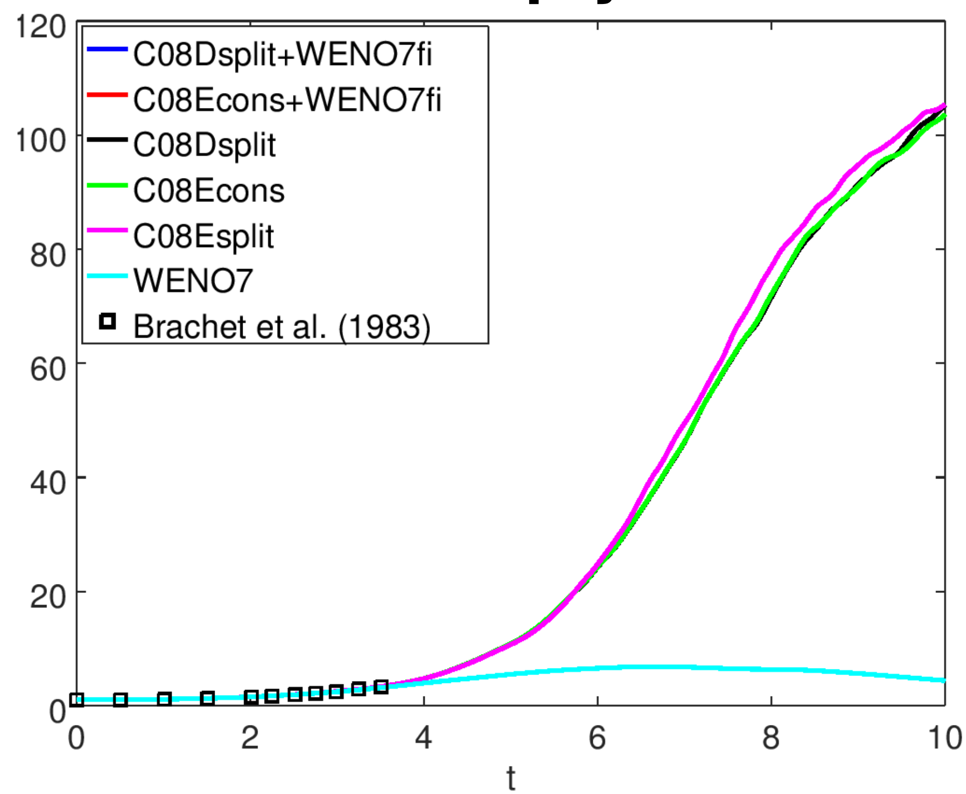


C08Dsplit+WENO7fi: 8^{th}-order central + Ducros et al. split +WENO7fi

C08Econs+WENO7fi: 8^{th}-order central entropy conservative flux + WENO7fi

C08Dsplit: 8^{th}-order central + Ducros et al. split

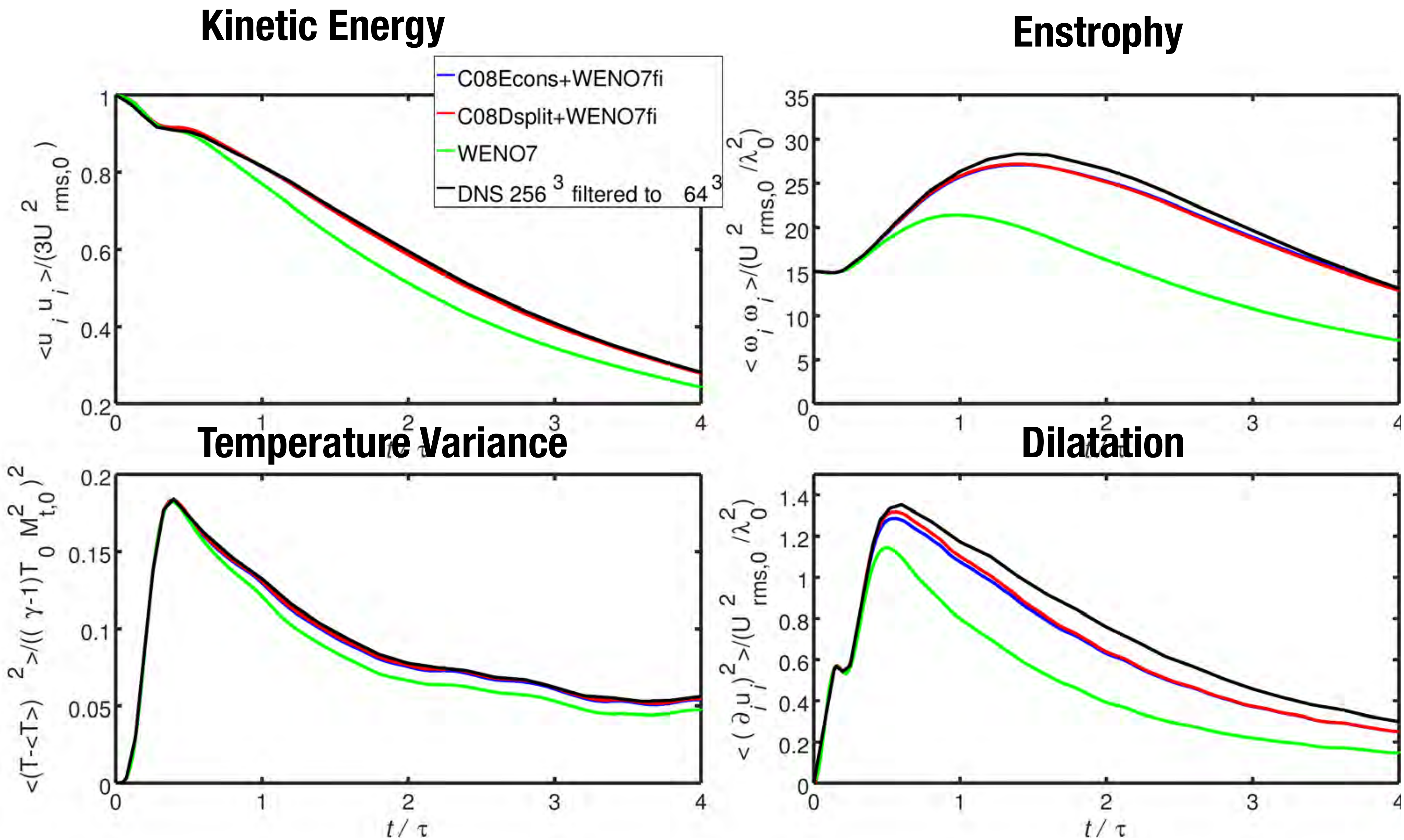
C08Econs: 8^{th}-order central Entropy conservative flux

C08Esplit: 8^{th}-order central + Entropy split

WENO7: Standard WENO7

3D Isotropic Turbulence with Shocklets

(Skew-Symmetric Splitting vs. Entropy Conservative Methods, 64^3 grids)

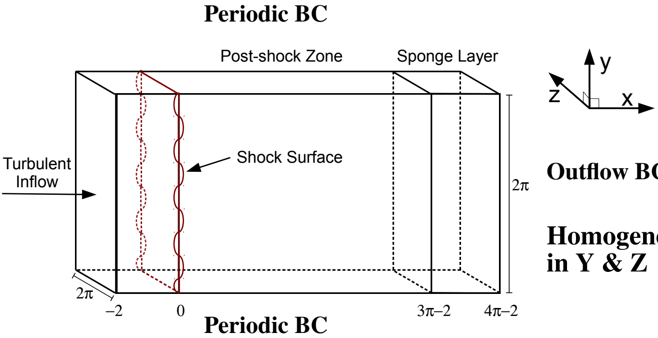


3D Shock-Turbulence Interaction Test Case

(Amplification of Turbulence Across a Supersonic Shock Wave: Supersonic flow over wings, fins, control surfaces & inlets)

What is needed:

- **Inflow BC:** **DNS of isotropic turbulence** *(from Larsson & Lele, Phys. Fluid, 2009)*
- **Sponge layer** **reduce domain size**
- **Compute back pressure** **to obtain mean stationary shock**



Outflow BC

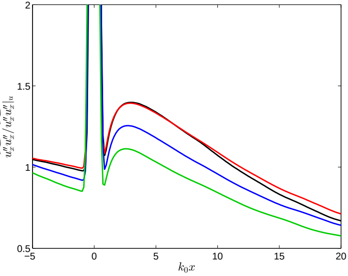
Homogeneous in Y & Z

Sponge source term: $W = -\frac{k_0 u_0}{2\pi}\left(\frac{x - x_{sp}}{x_{max} - x_{sp}}\right)(f - < f >_{yz})$

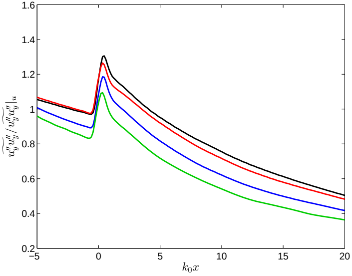
(Gently drive the flow towards a laminar state)

CDNS: Scheme Comparison, 389×64^2, $M = 1.5$

Streamwise Reynolds Stress



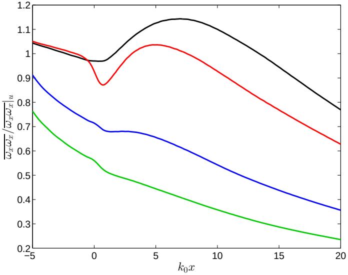
Streamwise Vorticity



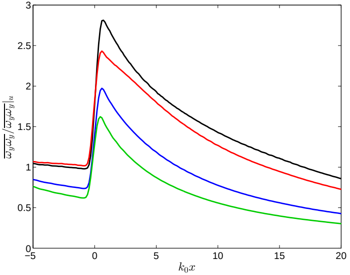
Filtered DNS
WENO7fi+split
WENO7
WENO5

All: No LES Model

Streamwise Vorticity



Transverse Vorticity



WENO7fi+splt:

- 8^{th}-order central & Ducros split
- 7^{th}-order WENO filter, **diss. in 3D**
- Ducros et al. sensor, **D = 0.01**

Subcell Resolution (SR) Method

Wang, Shu, Yee, & Sjögreen, 2012, JCP

Basic Approach

- Any high resolution shock capturing operator can be used in the convection step

  Test case: **WENO5, WENO7,** Roe flux, **RK4**
- Any standard shock-capturing scheme produces a few transition points in the shock

  ⇒ Solutions from the convection operator step, if applied directly to the reaction operator step, result in wrong shock speed

New Approach

Apply Subcell Resolution *(Harten 1989; Shu & Osher 1989)* **to the solution from the convection operator step before the reaction operator step**

Note: Subcell resolution methods can be used for LES using dynamic SGS model with shocks by locating the shock location & solve left & right problems

New Approach: Subcell Resolution Method for Stiff Source
(Obtaining Correct Shock/Contact/Shear Locations)

Selected Illustration: **Detonation**

More Complicated Examples & Minimizing Spurious Numerics:

Yee et al., Wang et al. and Kotov et al. (2002-2016)

1D C-J Detonation Wave

(Helzel et al. 1999; Tosatto & Vigevano 2008)

Left state (totally burned gas)	Right state (totally unburned gas)

$$\begin{pmatrix}\rho_b\\ u_b\\ p_b\end{pmatrix}=\begin{pmatrix}\rho_u\dfrac{[p_b(\gamma+1)-p_u]}{\gamma p_b}\\ S_{CJ}-(\gamma p_b/\rho_b)^{1/2}\\ -b+(b^2-c)^{1/2}\end{pmatrix}$$

$$\begin{pmatrix}\rho_u\\ u_u\\ p_u\end{pmatrix}=\begin{pmatrix}1\\ 0\\ 1\end{pmatrix}$$

$$S_{CJ}=[\rho_u u_u+(\gamma p_b \rho_b)^{1/2}]/\rho_u$$

$$b=-p_u-\rho_u q_0(\gamma-1) \qquad c=p_u^2+2(\gamma-1)p_u\rho_u q_0/(\gamma+1)$$

Ignition temperature $T_{ign}=25$

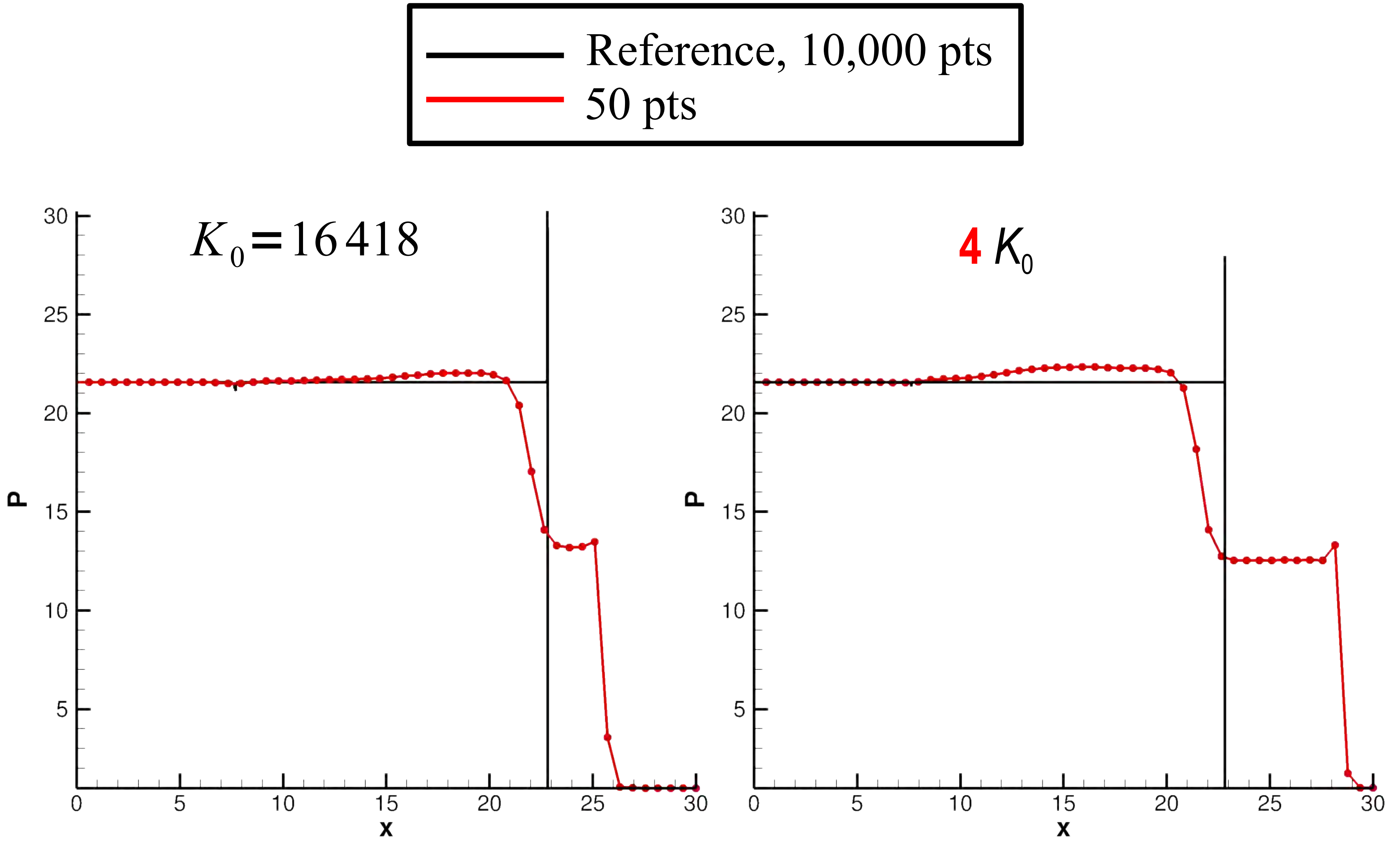
Heat release $q_0=25$

Rate parameter $K_0=16418$

$$K(T)=K_0\exp\left(\frac{-T_{ign}}{T}\right)$$

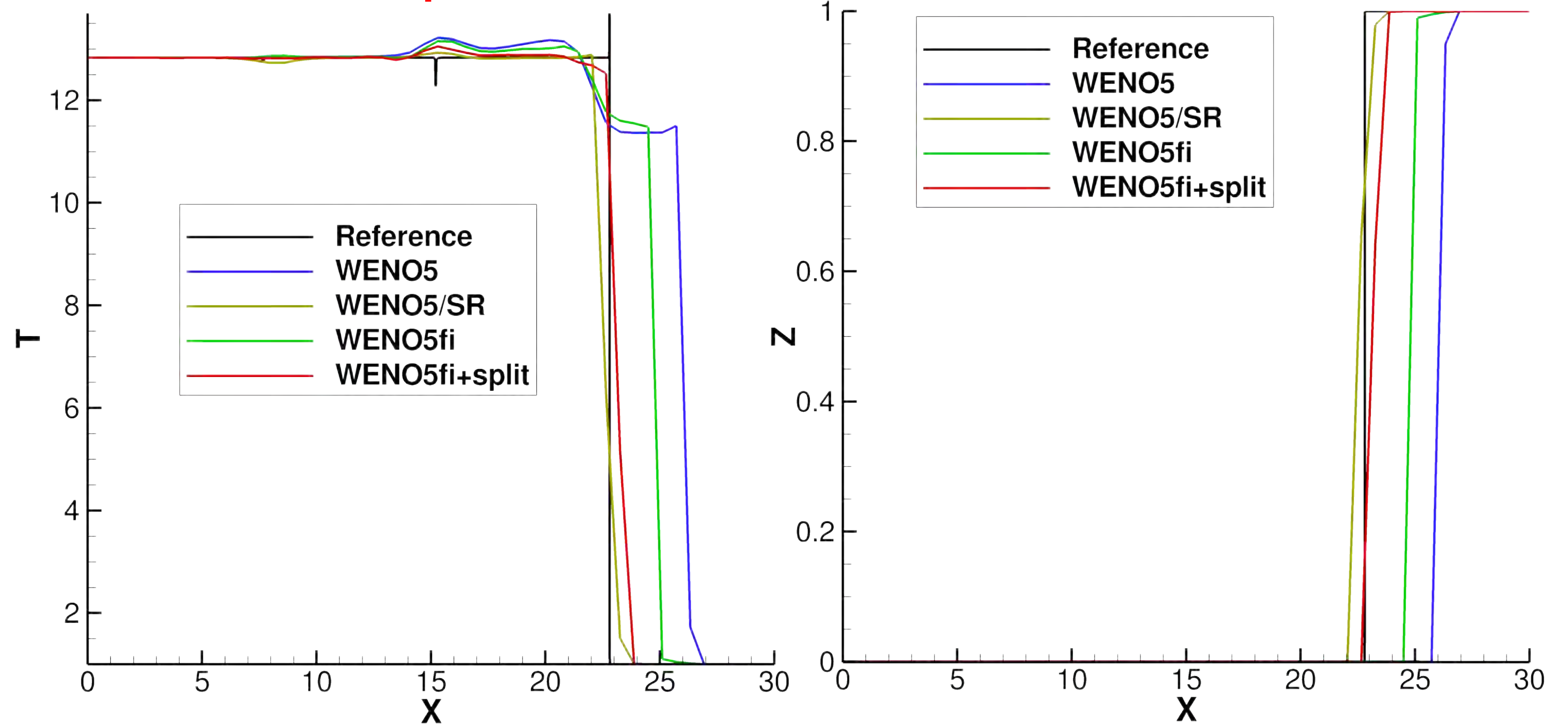
Wrong Propagation Speed of Discontinuities

(WENO5, Two Stiff Coefficients, 50 pts)



1D C-J Detonation (K_0 = 16418, 50 pts)

tend = 1.7



Standard Meth. – **WENO5:** Standard 5^{th} order WENO (WENO7, TVD)

Improved Meth. –
- **WENO5/SR:** WENO5 + subcell resolution
- **WENO5fi:** filter version of WENO5
- **WENO5fi+split:** WENO5fi + preprocessing (Ducros splitting)

Reference: WENO5, 10,000 points

(Strang Splitting & Safeguard)

Summary

(Split Centered Schemes & Entropy Conservative Centered (EC) Methods)

GAS dynamics:

- Split centered schemes can improve nonlinear stability for smooth flows in general
- Nonlinear filter version of split schemes can improve stability & accuracy for DNS & LES
- High order entropy conserving methods (centered or nonlinear filter version) provide similar stability & accuracy improvement as split schemes

Plasma:

- Split centered schemes can improve nonlinear stability in general for smooth flows but MHD equations dependent
- Nonlinear filter version of split schemes can improve stability & accuracy for flows with discontinuities but MHD equations dependent
- High order entropy conserving methods (centered or nonlinear filter version) can provide different stability & accuracy improvement, depending on the forms of the MHD equations & the choice of entropy fluxes

Backup Slides

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Ducros et al. Splitting

(Improve nonlinear stability for high order central schemes)

Split the derivative of a product into conservative & non-conservative parts:

$$(ab)_x = \frac{1}{2}(ab)_x + \frac{1}{2}ab_x + \frac{1}{2}a_x b$$

Approximation of the split form can be written in conservative form: e.g.,

$$\frac{1}{2}D_0(ab)_j + \frac{1}{2}a_j D_0 b_j + \frac{1}{2}b_j D_0 a_j = \frac{1}{4}D_+(a_j + a_{j-1})(b_j + b_{j-1})$$

D_0: 2nd-order central, $D_+ u_j = (u_{j+1} - u_j)/\Delta x$

The above can be generalized to $2p^{th}$-order accurate: *Ducros et al. 2000*

$$D_{0p}u_j = \sum_{k=1}^{p} \alpha_k^{(p)} D_0(k)u_j \qquad D_0(k)u_j = (u_{j+k} - u_{j-k})/(2k\Delta x)$$

$$\sum_{k=1}^{p} \alpha_k^{(p)} = 1 \qquad \sum_{k=1}^{p} \alpha_k^{(p)} k^{2n} = 0, \;\; n = 1, \ldots, p-1$$

Ducros et al. Splitting (Cont.)
(Improve nonlinear stability for high order central schemes)

Approximation of the 2p^th-order split form in conservation form:

$$\frac{1}{2}D_p(ab)+\frac{1}{2}D_p(a)b+\frac{1}{2}aD_p(b)=$$

$$\frac{1}{\Delta x}\sum_{k=1}^{p}\frac{1}{2}\alpha_k\left((a_{j+k}b_{j+k}-a_{j-k}b_{j-k})+a_j(b_{j+k}-b_{j-k})+(a_{j+k}-a_{j-k})b_j\right)$$

$$=\frac{1}{\Delta x}\sum_{k=1}^{p}\frac{\alpha_k}{2}\left(\sum_{m=0}^{k-1}(a_{j-m}+a_{j+k-m})(b_{j-m}+b_{j+k-m})\right.$$

$$\left.-\sum_{m=0}^{k-1}(a_{j-1-m}+a_{j-1+k-m})(b_{j-1-m}+b_{j-1+k-m})\right)=\frac{1}{\Delta x}(h_{j+1/2}-h_{j-1/2})$$

High Order Methods with Subcell Resolution

Strang Splitting + Subcell Resolution (SR)

$$U_t + F(U)_x + G(U)_y = S(U)$$

Convective step

$$U_t + F(U)_x + G(U)_y = 0$$

$A \to U^*$

Convective difference operator

(Full time step of WENO5 or WENO7, RK4)

SR step

$SR \to U^{**}$

SR operator

(No time involved)

Reactive step

$$\frac{dU}{dt} = S(U)$$

$R \to U^{n+1}$

Reaction difference operator

(RK1, RK2, RK3, RK4)

Numerical solution: $U^{n+1} = A^*\left(\frac{\Delta t}{2}\right) R(\Delta t) A^*\left(\frac{\Delta t}{2}\right) U^n$
(At the next time level)

OR: $U^{n+1} = A^*\left(\frac{\Delta t}{2}\right) R\left(\frac{\Delta t}{N_r}\right) \cdots R\left(\frac{\Delta t}{N_r}\right) A^*\left(\frac{\Delta t}{2}\right) U^n$

A^* operator includes SR step correction at shocks
N_r – number of subiterations

Nonlinear Filter Step $(U_t + F_x(U) = 0)$

- **Denote the solution by the base scheme (e.g. 6^{th} order central, $4th$ order RK)**

$$U^* = L^*(U^n)$$

- **Solution by a nonlinear filter step**

$$U_j^{n+1} = U_j^* - \frac{\Delta t}{\Delta x}\left[H_{j+1/2} - H_{j-1/2}\right]$$
$$H_{j+1/2} = R_{j+1/2}\overline{H}_{j+1/2}$$

$\overline{H}_{j+1/2}$ **- numerical flux,** $R_{j+1/2}$ **- right eigenvector, evaluated at the Roe-type averaged state of** U_j^*

- **Elements of** $\overline{H}_{j+1/2}$**:**

$$\overline{h}_{j+1/2} = \frac{\kappa_{j+1/2}^m}{2}\left(s_{j+1/2}^m\right)\left(\phi_{j+1/2}^m\right)$$

$\phi_{j+1/2}^m$ **- *Dissipative portion of a shock-capturing scheme***
$s_{j+1/2}^m$ **- *Local flow sensor (indicates location where dissipation needed)***
$\kappa_{j+1/2}^m$ **- *Controls the amount of*** $\phi_{j+1/2}^m$

Improved High Order Filter Method

Form of nonlinear filter

$$\bar{h}_{j+1/2} = \frac{\kappa^m_{j+1/2}}{2}\left(s^m_{j+1/2}\right)\left(g^m_{j+1/2} - b^m_{j+1/2}\right)$$

Control amount of dissipation based on local flow condition

Local flow sensor *(Shock Sensor, ACM (Harten), Ducros et al, Multiresolution wavelet, etc.)*

Any High Order Shock capturing numerical flux *(e.g. WENO7)*

High order central numerical flux *(e.g. 8th order central)*

2007 – κ = global constant
2009 – $\kappa_{j+1/2}$ = local, evaluated at each grid point
Simple modification of κ *(Yee & Sjögreen, 2009)*

$$\kappa = f(M)\cdot\kappa_0$$

$$f(M) = min\left(\frac{M^2}{2}\frac{\sqrt{4+(1-M^2)^2}}{1+M^2}, 1\right)$$

For other forms of $\kappa_{j+1/2}, s_{j+1/2}$, see *(Yee & Sjögreen, 2009)*